SUPPORTING INFORMATION

Title: Inducing Spin Crossover in Amphiphilic Iron(III) Complexes
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1. Magnetic data
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1. Magnetic Data

$[FeL_H]BF_4$, $C_{20}H_{24}BF_4FeN_4O_2$, 1.

H = 1500 and 5000 G (1500 G to 75 K; 5000G above 75 K. No dependence on H.)
MW = 495.1 Da
Mass = 25.37 mg
DC = -244 cm^3mol^{-1}

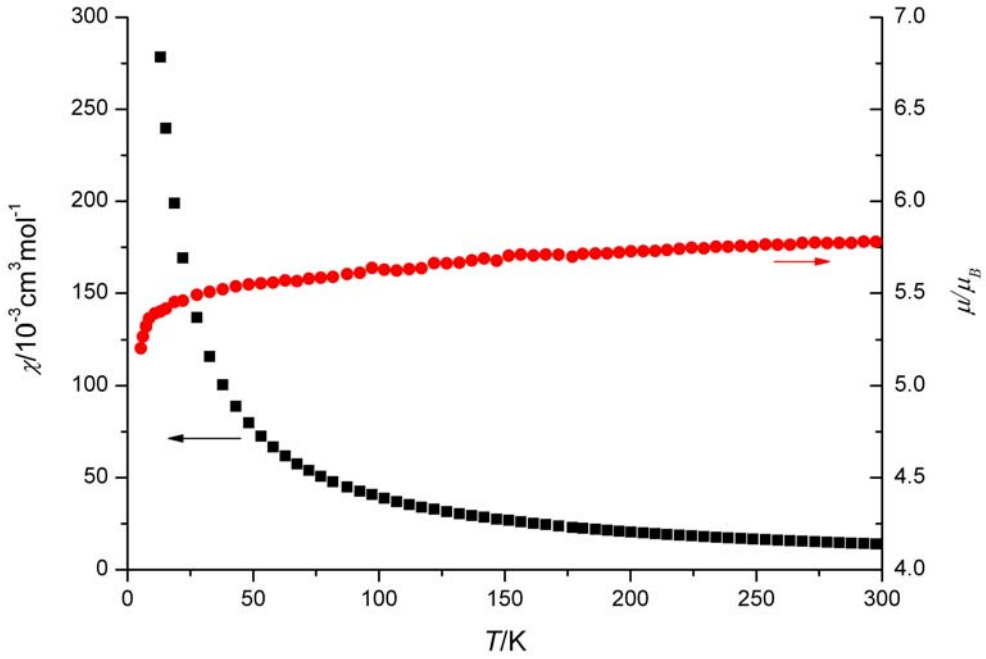

Figure S1. Variable temperature magnetic susceptibility and magnetic moment of $[FeL_H]BF_4$.

Magnetic data

Table S1. magnetic data for **1**

T/K	10^6 χ/cm^3mol^{-1}	μ/BM
5.3	643067	5.204
6.2	558236	5.268
7.4	477443	5.322
8.6	417430	5.363
10.9	333747	5.39
13.1	278438	5.401
15.3	239700	5.416

18.7	198925	5.452
22	169221	5.459
27.6	136764	5.491
32.7	115972	5.507
37.9	100564	5.521
43.1	88863	5.537
48.2	79844	5.548
53.1	72631	5.553
57.9	66719	5.558
62.7	61870	5.569
67.4	57497	5.566
72.1	54014	5.579
76.9	50675	5.584
81.7	47806	5.589
87.3	44958	5.604
92.4	42602	5.611
97.2	40897	5.637
102.1	38786	5.628
107	36943	5.623
112	35397	5.631
116.9	33980	5.636
121.9	32896	5.663
126.9	31588	5.662
132	30417	5.666
136.9	29434	5.678
141.8	28538	5.689
146.8	27447	5.676
151.6	26840	5.704
156.4	26059	5.71
161.4	25214	5.705
166.3	24513	5.71
171.4	23775	5.709
176.9	22962	5.699
181	22562	5.714
186	21955	5.715
190.7	21420	5.716
195.5	20942	5.722
200.2	20486	5.728
205.1	20008	5.729
209.8	19569	5.73
214.5	19172	5.735
219.4	18783	5.741
224.3	18412	5.747
229.2	18004	5.744
234	17681	5.753
238.8	17325	5.753
243.8	17002	5.757
248.6	16650	5.754
253.6	16387	5.765
258.5	16067	5.763
263.4	15769	5.763
268.3	15529	5.773
273.3	15260	5.775
278.2	14977	5.772
283	14726	5.773

287.8	14481	5.773
292.7	14271	5.78
297.5	14036	5.779

$[FeL_{C6}]BF_4$, $C_{32}H_{48}BF_4FeN_4O_2$, 2.

H = 3000 - 8000 G
MW = 663.4 Da
Mass = 14.38 mg
DC = -386 cm^3mol^{-1}

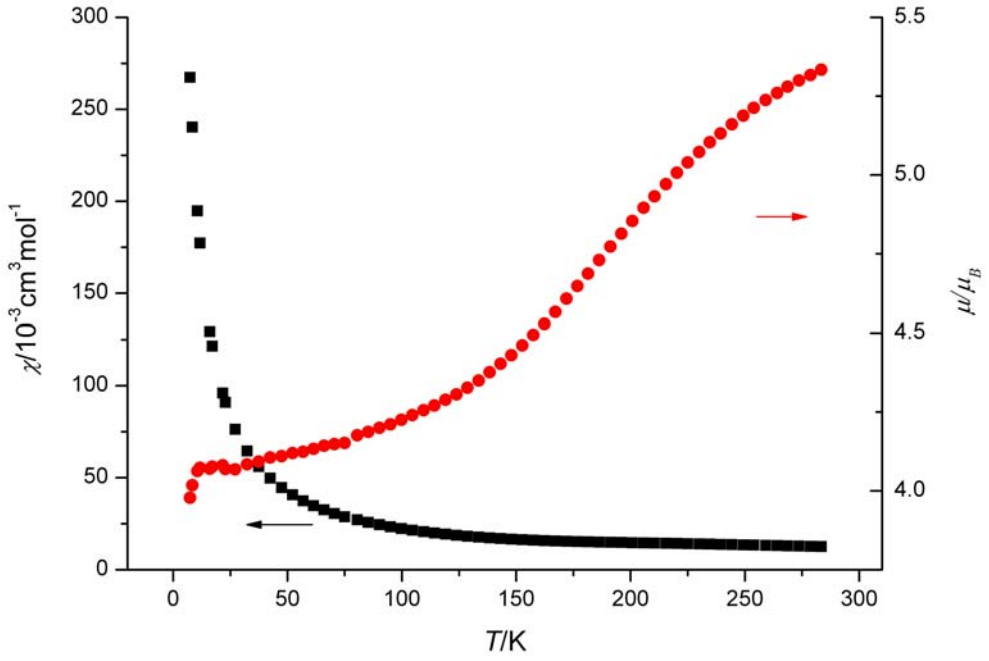

Figure S2. Variable temperature magnetic susceptibility and magnetic moment of $[FeL_{C6}]BF_4$.

Magnetic data

Table S2. magnetic data for **2**

T/K	10^6 χ/cm^3mol^{-1}	μ/BM
7.4	267405	3.978
8.4	240297	4.018
10.6	194763	4.063
11.7	177298	4.073
16	129452	4.07
17.1	121547	4.077
21.7	96024	4.081
22.8	90989	4.069
27.1	76336	4.068
32.3	64570	4.084
37.4	56010	4.093
42.4	49708	4.106

47.4	44563	4.11
52.2	40656	4.12
56.8	37432	4.124
61.4	34782	4.133
66	32515	4.143
70.5	30520	4.148
75	28744	4.152
79.6	27242	4.164
80.5	27086	4.176
84.5	25776	4.174
85.3	25700	4.187
89.2	24528	4.183
90.2	24456	4.2
93.9	23444	4.196
95	23345	4.211
98.5	22452	4.206
99.8	22369	4.225
104.6	21493	4.24
109.5	20680	4.256
114.2	19968	4.271
119.1	19312	4.289
123.9	18714	4.306
128.7	18190	4.327
133.6	17714	4.35
138.4	17297	4.376
143.2	16925	4.403
147.9	16592	4.43
152.7	16293	4.461
157.5	16036	4.494
162.3	15803	4.529
167.1	15598	4.566
172	15435	4.608
176.8	15278	4.648
181.4	15143	4.687
186.3	15018	4.73
191.2	14900	4.773
196	14782	4.814
200.8	14670	4.854
205.7	14570	4.896
210.5	14452	4.932
215.5	14337	4.971
220.3	14229	5.007
225	14115	5.04
230	13990	5.073
234.7	13878	5.104
239.4	13757	5.132
244.3	13635	5.161
249.3	13500	5.188
253.9	13385	5.213
259.1	13239	5.238
264.1	13100	5.26
268.7	12972	5.28
273.7	12833	5.3
278.7	12683	5.317
283.4	12551	5.334

$[FeL_{C12}]BF_4$, $C_{44}H_{72}BF_4FeN_4O_2$, 3

H = 8000 G
MW = 831.71 Da
Mass = 20.81 mg
DC = -532 cm^3mol^{-1}

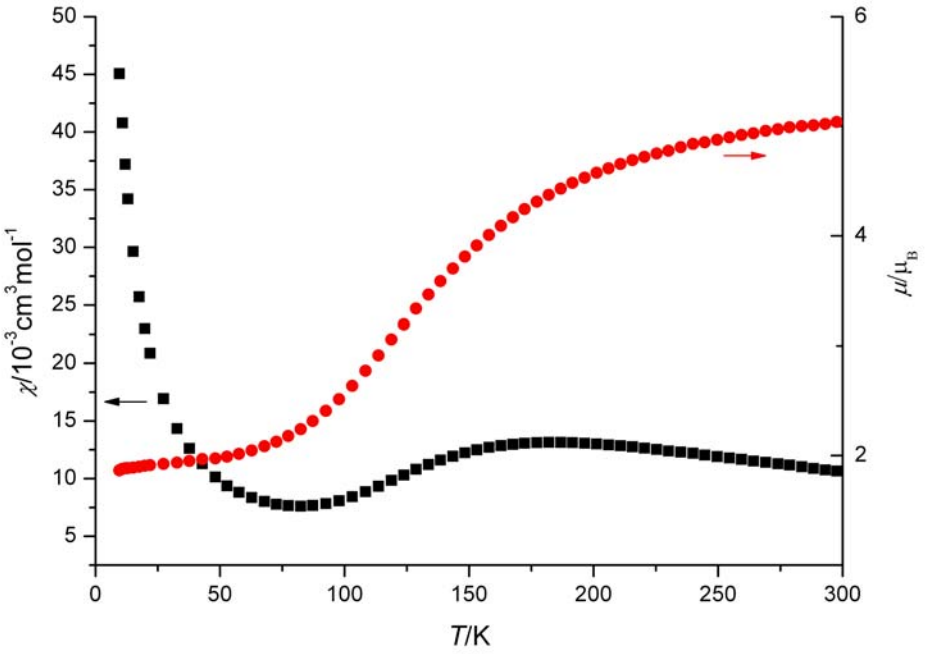

Figure S3. Variable temperature magnetic susceptibility and magnetic moment of $[FeL_{C12}]BF_4$.

Magnetic data

Table S3. magnetic data for **3**

T/K	10^6 χ/cm^3mol^{-1}	μ/BM
9.6	45063	1.865
10.8	40798	1.879
11.9	37205	1.884
13	34206	1.886
15.1	29642	1.89
17.5	25720	1.898
19.8	23010	1.907
21.9	20870	1.913
27.3	16939	1.924
32.7	14337	1.936

37.7	12622	1.951
42.9	11290	1.968
48.1	10147	1.975
52.8	9376	1.99
57.6	8818	2.016
62.7	8360	2.047
67.8	8026	2.086
72.6	7784	2.126
77.4	7667	2.179
82.4	7618	2.241
87.2	7681	2.315
92.5	7838	2.409
97.8	8087	2.515
103.1	8439	2.637
108.4	8873	2.774
113.6	9343	2.914
118.8	9852	3.059
123.8	10315	3.195
128.7	10815	3.337
133.7	11231	3.465
138.5	11612	3.587
143.5	11942	3.702
148.3	12241	3.811
153.1	12498	3.912
158	12716	4.008
162.8	12863	4.092
167.6	12978	4.17
172.3	13068	4.244
177.2	13123	4.312
182	13147	4.374
186.8	13143	4.431
191.5	13125	4.484
196.4	13069	4.531
201.2	13014	4.576
206	12929	4.616
210.8	12858	4.656
215.6	12764	4.691
220.4	12646	4.721
225.3	12537	4.752
230.1	12398	4.777
235	12305	4.809
239.9	12205	4.839
244.6	12045	4.854
249.6	11913	4.877
254.5	11793	4.899
259.4	11673	4.921
264.2	11532	4.936
269.1	11420	4.958
274	11288	4.973
278.7	11177	4.991

283.6	11031	5.002
288.3	10885	5.009
293	10760	5.021
297.6	10665	5.039

2. Short Contacts in 2

No evidence for hydrogen-bonding, anion-π interactions or π-π interactions was detected in either **1** or **2**. Short contacts between the alkyl chains and between the alkyl chains and BF_4^- counterions in **2** are tabulated below:

Table S4: Short contacts around site 1 (Fe1, HS) for **2**

C2	C51	3.53
C4	C33	3.42
C4	C38	3.30
C4	C52	3.69
C6	C62	3.45
C7	C62	3.53
C8	F6	3.10
C10	F6	3.18
C11	F6	3.24
C12	C46	3.63
C12	C47	3.70
C25	C64	3.66
C26	C64	3.72
C32	C57	3.77

Table S5: Short contacts around site 2 (Fe2, SCO) for **2**

C33	C4	3.42
C38	C4	3.30
C42	F1	3.15
C43	F2	3.02
C45	F3	3.22
C46	C12	3.63
C47	C12	3.70
C51	C2	3.53
C52	C4	3.69
C53	F2	3.40
C57	C32	3.77
C62	C6	3.45
C62	C7	3.53
C64	C25	3.66
C64	C26	3.72

3. Packing diagrams for 1 and 2

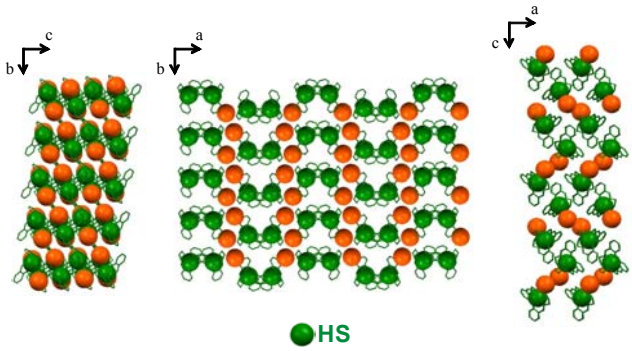

Figure S4. Packing diagram of $[FeL_H]BF_4$, **1**, at 293 K (orange – BF_4^- counterions).

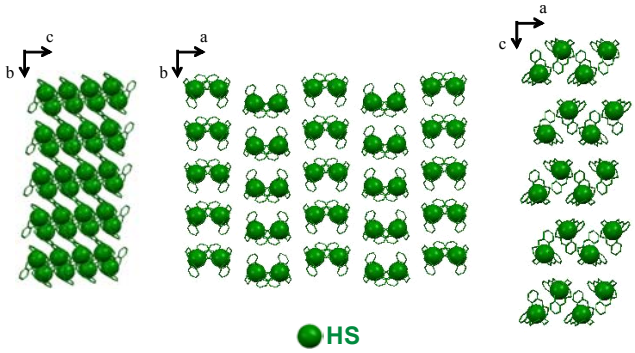

Figure S5. Packing diagram of $[FeL_H]BF_4$, **1**, at 293 K without BF_4^- counterions

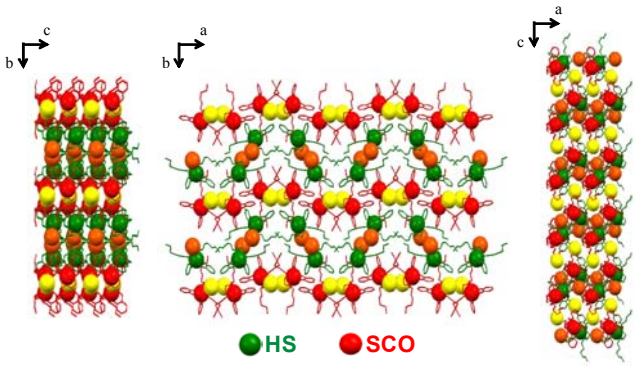

Figure S6. Packing diagram of $[FeL_{C6}]BF_4$, **2**, at 100 K (yellow and orange – BF_4^- counterions)

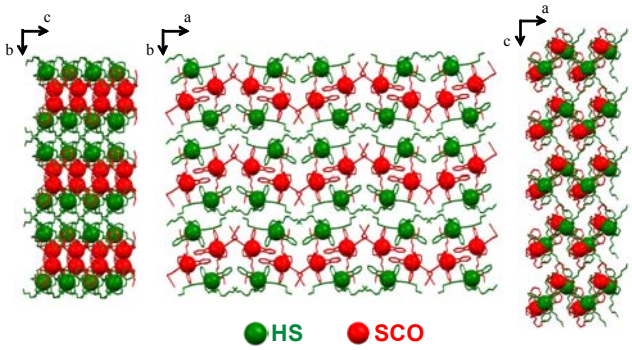

Figure S7. Packing diagram of $[FeL_{C6}]BF_4$, **2**, at 100 K without BF_4^- counterions